

MEMORANDUM

Date: 3/23/2006

SUBJECT: Dietary Risk Assessment for Alkylbenzene Sulfonates

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PC CODES: 079010 Sodium dodecylbenzene sulfonic acid
098002 Dodecylbenzene sulfonic acid
190116 C10-16-Alkylbenzene sulfonic acid

DP BARCODES: D327731

DECISION #: 362580

Alkylbenzene Sulfonate Dietary Exposure

The Registration Eligibility Document (RED) covers the potential dietary exposure to the active ingredient(s) sodium dodecylbenzene sulfonate, dodecylbenzene sulfonate and benzene sulfonic acid. This RED does not address the dietary exposure that will result from the use of products containing these chemicals as inert ingredients. Chemicals classed as any of these chemicals are being considered together because chemicals named dodecylbenzene sulfonate actually contain alkylbenzene sulfonates in addition to dodecylbenzene sulfonate. Labeling modifications will be made to these chemicals as a result of the reregistration process.

The uses for these chemicals include: (1), food handling/storage establishments, premises and equipment; (2) agricultural premises and equipment; and (3) fruit and vegetable rinses.

The 21 CFR 178.1010 Regulation for sanitizing solutions read:

Dodecylbenzene sulfonate: 178.1010(b)(7) and 178.1010(c)(5).

The site reads: “In addition to use on food-processing equipment and utensils, this solution may be used on glass bottles and other glass containers intended for holding milk”. The use limitation for the chemical is 400 ppm.

Dodecylbenzene sulfonic acid: 178.1010 (b)(10) and 178.1010 (c)(7).

The site reads: “In addition to use on food-processing equipment and utensils, this solution may be used on beverage containers except milk containers or equipment”. The use limitation is 400 ppm.

Sodium dodecylbenzenesulfonate: 178.1010(b)(21) and 178.1010(c)(16).

The site reads, “In addition to use on food processing equipment and utensils this solution can be used on glass bottles and other glass containers intended for holding milk”. The use limitation is 430 ppm equivalent to ~ 400ppm of the free acid.

Dodecylbenzene sulfonic acid; 178.1010(b)(40) and 178.1010(c)(35).

The site reads: “In addition to use on food-processing equipment and utensils, this solution may be used on dairy processing equipment”. The use limitation is 5.5 ppm.

It appears that dodecylbenzenesulfonic acid solutions containing up to 400 ppm can be used on glass bottles and containers containing milk but cannot be used on dairy processing equipment at this level. The registrant and user may have difficulty in distinguishing between glass-lined equipment and glass containers.

These 21 CFR citations do not specifically state that the solutions may be used on food contact articles including dishes, pots and pans, glasses etc. However, there are many labels registered for use on these sites.

The 40 CFR 180 Regulation reads:

Tolerance Exemption Expression/ Chemical Name	CAS No.	PC Code	40 CFR 180.	Use Pattern (Pesticidal)	Active Products
Benzenesulfonic acid, dodecyl-	27176-87-0	098002	940 (b)	food contact sanitizing solutions for dairy processing equipment, and food processing equipment and utensils; end use concentration not to exceed 5.5 ppm	18
			940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 400 ppm	
Benzenesulfonic acid dodecyl-, sodium salt	25155-30-0	079010	940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 430 ppm	3

The RMB II Chemical Review Manager should ascertain the correct use sites and limitations for these chemicals.

Many of the labels include uses for the sanitization of food serving equipment, glasses, dishes, utensils and pots and pans. These surfaces that have been treated with the dodecylbenzene sulfonate products may bear small residues of the dodecylbenzene sulfonate. Residues from treated surfaces can migrate to food coming into contact with the treated surfaces and can be ingested by humans.

The maximum label rates for the dodecylbenzene sulfonates are 400 ppm for use in antimicrobial formulations (Food contact surface sanitizing solutions).

The maximum rate for dodecylbenzene sulfonates in sanitizer end-use solutions is 400 ppm except for dairy processing equipment. Uses on food processing equipment are discussed below under “Food Processing Industry”.

FOOD CONTACT SURFACES IN THE FOOD SERVICE INDUSTRY

AD will use the 400 ppm level permitted in an end use solution in our calculations.

In the absence of residue data for residues of dodecylbenzene sulfonate on treated food contact surfaces reflecting the registered use patterns, the Agency can calculate residue levels that may occur in food from the application rates on food contact surfaces.

To estimate the Estimated Daily Intake (EDI), the Agency has used the following model calculation. This model is taken from FDA Guidelines.

The maximum ingredient percentage for dodecylbenzene sulfonates registered for use in food handling establishments in kitchens, cafeterias, supermarkets and meat and poultry plants is 400 ppm).

$$\text{EDI} = (1 \text{ mg/cm}^2) \times \text{wt. fraction of wash solution (AR)} \times \text{SA} \times \text{FMF} / \text{BW}$$

Where:

AR = Application rate

SA = surface to which food is exposed, assume 4000 cm^2

FMF = Fraction of pesticide migrating to food, assume 100%*

BW = 70 for male adults, 60 kg for female adults and 15 kg for children

$$\begin{aligned} \text{EDI from the FDA model} &= 400 \text{ } \mu\text{g}/1000 \text{ mg (ppm)} \times 1.0 \text{ mg/cm}^2 \times 4000 \text{ cm}^2 \\ &\text{/person/day} \\ &= 1600 \text{ } \mu\text{g dodecylbenzene sulfonate/person/day} \end{aligned}$$

Assuming that an average adult consumes 3000 gm of food per day,

$$\text{Then } 1600 \text{ } \mu\text{g a.i./3000 gm food} = 0.53 \text{ } \mu\text{g a.i./gm (ppm) of food}$$

This calculation reduces the dietary consumption to μg of a.i. per gm of food.

Assume that an adult consumes 3000 gm of food /day

$$1600 \text{ } \mu\text{g a.i./70 kg BW} = 22.9 \text{ } \mu\text{g dodecylbenzene sulfonate/kg/day for a male adult}$$

$$1600 \text{ } \mu\text{g a.i./60 kg BW} = 26.7 \text{ } \mu\text{g dodecylbenzene sulfonate/kg/day for a female adult}$$

Assuming that a child consumes 1500 gm of food per day,

$$\text{Then: } 0.53 \text{ } \mu\text{g a.i./gm (ppm) of food} \times 1500 = 795 \text{ } \mu\text{g a.i./day}$$

$$800 \text{ } \mu\text{g a.i./15 kg BW} = 53 \text{ } \mu\text{g dodecylbenzene sulfonate/kg/day for child}$$

FOOD CONTACT SURFACES IN THE FOOD PROCESSING INDUSTRY

The 21 CFR 178.1010 Regulations and the 40 CFR 940 Regulations do not specifically permit the use on milk processing equipment at a level of 400 ppm.

However, the labels include uses for the sanitization of food processing equipment such as tanks, pipelines, evaporators, filters, pasteurizers, aseptic equipment including dairies, wineries, breweries and beverage plants, meat and poultry processing/packing plants, milk and dairy products /packing plants, seafood and vegetable processing/packing plants, food processing/packing plants and egg processing/packing equipment surfaces. These uses would permit the sanitization of the interior of food processing and storage equipment.

This use could be additive to the treatment of food contact surfaces such as glasses, dishes, utensils and pots and pans.

AD will use an FDA model to estimate residues that could transfer from treated surfaces to food from this type of use.

According to the FDA, the exposure estimates for this type of use can be calculated using the milk truck model that is described in the FDA document, “Sanitizing Solutions: Chemistry Guidelines For Food Additive Petitions”, pages 9-10.

This guidance states on page 9, “For applications limited to use of the food sanitizer on food processing equipment and utensils, the Agency has determined that estimates of sanitary exposure from use in dairy processing plants significantly exceed estimates based on other uses with food processing equipment and utensils. Depending on the available safety data, the petitioner may either submit a petition for the broader use of its sanitizer on “food processing equipment and utensils including dairy processing plants” or for the more limited use on “food processing equipment and utensils excepting use in dairy processing plants.”

The next paragraph of the document states, “The following simplified example will illustrate the calculation of the EDI of residual sanitizer solution in milk from sanitizer use in a dairy processing plant. Although in practice consideration of all of the components of a milk handling system must be included as sources of sanitizer residue in milk, for this example the only source is assumed to be a sanitized tank truck to transport the milk. It is further assumed that the milk undergoes no additional dilution prior to reaching the consumer. Assuming a cylindrical model for the tank truck (4000 gallon capacity) with a length of 19.9 feet and cross-sectional diameter of 6 feet, and an internal surface area of 413 sq ft is calculated for the tank. Assuming that the sanitizer treatment leaves a residue of 1 mg/sq cm and the ‘at use’ concentration of component X is 200 ppm, the concentration of X in the milk residing in the tank would equal:

413 sq ft/1 truck x 1truck/4000gal x 1 mg/sq cm x 200 µg/1000 mg x 929 sq cm/1 sq ft x 0.264 gal/1L = 5.1 µg x/L milk ~ 5.1 ppb”.

The maximum application rate for the dodecylbenzene sulfonate chemicals in food processing equipment is 400 ppm.

Then using the FDA model, residues resulting in milk from the use would be calculated as:

413 sq ft/1 truck x 1truck/4000gal x 1 mg/sq cm x 400 µg/1000 mg x 929 sq cm/1 sq ft x 0.264 gal/1L = 5.1 µg x/L milk ~ 10.1 ppb.

If an adult were to consume 3000 gm of food per day containing 10.1µg/L or 10.1µg/kg (1000 gm), then the person would ingest 30.4 µg of dodecylbenzene sulfonate per day.

A child consuming 1500 gm of food per day would consume would ingest 15.2 µg of dodecylbenzene sulfonate per day.

DIETARY EXPOSURE ASSESSMENT FOR THE FOOD SERVICE AND FOOD PROCESSING INDUSTRIES

TABLE 1

Cumulative Estimated Dietary Intake of LAS

Use	Dietary Conc. (ppb)	Estimated Daily Intake (µg/person/day)	Daily Dietary Dose (mg/kg bw/day)
Food Service Industry	0.53 ppb	1600 (adult M) 1600 (adult F) 800 (child)	0.023 (adult M) 0.027 (adult F) 0.053 (child)
Food Processing Industry	10.1 ppb	30.3 (adult M) 30.3 (adult F) 15.1 (child)	0.00043 (adult M) 0.00050 (adult F) 0.001 (child)
Cumulative	12.6 ppb	1630.3 (adult M) 1630.3 (adult F) 815.1 (child)	0.023 (adult M) 0.027 (adult F) 0.054(child)

There were no effects attributable to a single dose for the acute dietary risk (Deborah Smegal memo.

Utilizing the chronic RfD or cPAD of 0.5 mg/kg/day taken from the Deborah Smegal memo, the dietary risks were estimated in Table 2 below.

$$\% \text{ PAD} = \text{exposure/PAD} \times 100$$

TABLE 2
Dietary Risks of LAS

USE	DAILY DIETARY DOSE (mg/kg bw/day)	% aPAD	% cPAD
Food Service Industry	0.023 (adult M)	No effects	4.6%
	0.027 (adult F)	No effects	5.4%
	0.053 (child)	No effects	10.6%
Food Processing Industry	0.00043(adult M)	No effects	0.086%
	0.00050 (adult F)	No effects	0.1%
	0.001 (child)	No effects	0.2%
Cumulative	0.0234(adult M)	No effects	4.69%
	0.0275(adult F)	No effects	5.5%
	0.054(child)	No effects	10.8%

The food service and food processing industry uses do not result in dietary risks of concern.

FRUIT AND VEGETABLE WASH

The label, CS-100 Acid Anionic Sanitizer, EPA Reg. # 71695-1, bears a use for washing fruits and vegetables.

The FDA Regulation, 21 CFR 173.315, permits this use provided that the wash solution does not contain dodecylbenzene sulfonic acid at a level greater than 0.2%. No potable water rinse is required by the Regulation. We presume that the use limitation is for the parent chemical because the Regulation makes no mention of formulations. The use limitation states, “Not to exceed 0.2% in wash water. May be used in washing or to assist in the lye peeling of fruits and vegetables”. Note: If the use limitation were intended to apply to a formulation, there would be a broad range of application rates depending on the concentration of the chemical in the formulation.

The label bears a use that provides for a fruit and vegetable wash with a solution containing 0.16 % dodecylbenzene sulfonic acid, without a potable water rinse.

The label also bears a use a use that provides for a fruit and vegetable wash with a solution containing 0.31% dodecylbenzene sulfonic acid, with a potable water rinse.

There are no data to show that the level of residues on fruits and vegetables would be reduced to the level that would have occurred from a 0.2% wash. However, AD concludes that dodecylbenzene sulfonic acid residues would be significantly reduced by the potable water rinse and would be less than residues resulting from the 0.2% wash.

There are no residue data to show the level of dodecylbenzene sulfonic acid that will result on fruits and vegetables from the 0.2% wash solution with a potable water rinse.

Lacking residue data to show the level of residues expected on fruits and vegetables, we have calculated the level of residues on fruits and vegetables using the following model.

Dodecylbenzene sulfonate Fruit and Vegetable Wash Dietary Residue Calculations:

Calculation for percent dodecylbenzene sulfonate in the wash water:

The maximum use rate is 2000 ppm of dodecylbenzene sulfonate (0.2% x 10,000) for fruit and vegetables.

We will use the surface area and weight of Thompson Seedless grapes to calculate residues in fruits and vegetables. This is a small grape which accounts for half of the table grapes grown in California and is used to make over 90% of the grapes grown in the United States.

Grapes specifications:

Diameter of one grape = 16 mm

(Source: University of California Cooperative Extension, Tulare County

<http://cetulare.ucdavis.edu/pubgrape/tb195.htm>

Mass of one grape = 4.0 gm or 0.0040 kg

(Source: University of California Cooperative Extension, Tulare County

<http://cetulare.ucdavis.edu/pubgrape/tb195.htm>.)

Surface area of one grape = 15.88 cm²

Based on surface area of a sphere where $A = 4\pi r^2$ (where $r = 8$ mm)

$A = 4 \times 3.14 \times (8 \text{ mm})^2$

$A = 803.8 \text{ mm}^2$

$A = 8.04 \text{ cm}^2$

Amount of Residue on Grapes:

Assume the film thickness of the solution on the surface of the grape is 0.0023 g/cm²

(Source: Proctor and Gamble exposure assessment for ingestion of dishwashing product residues - based on the amt of rinse water in contact with dishware surfaces

http://www.scienceinthebox.com/en_UK/safety/ingestionfromsurface_en.html)

$0.0023 \text{ g/cm}^2 \times 8.04 \text{ cm}^2 \times 0.002$ (0.2%) dodecylbenzene sulfonate = 0.0000369 gm or 0.037 mg dodecylbenzenesulfonate

$0.037 \text{ mg dodecylbenzene sulfonate} / 0.004 \text{ kg grape} = 9.25 \text{ mg/kg or ppm}$

DIETARY EXPOSURE ASSESSMENT FOR THE FRUIT AND VEGETABLE WASH

This part of the non-cancer dietary risk assessment was carried out by Cassi Walls (RASSB/AD). It was conducted using the Dietary Exposure Evaluation Model (DEEM-FDIC™), Version 2.03 which uses food consumption data from the USDA's Continuing Surveys of Food Intake by Individuals (CSFII) from 1994-1996 and 1998. This assessment is Tier 1, conservative (assumes 100% crop treatment) and uses the deterministic approach. As input parameters for modeling analyses, the level of 9.25 ppm was used based on the modeling discussed above.

TABLE 3

Dietary Risk for Fruit and Vegetable Wash

USE	DAILY DIETARY DOSE (mg/kg bw/day)	% aPAD	% cPAD
Fruit and Vegetable Wash	0.0979 (U.S. Pop.)	No Effects	19.6%
	0.2793 (child 1-6)	No Effects	55.9%
	0.3558 (child 1-2)	No Effects	71.2%
	0.2573 (child 3-5)	No Effects	51.5%

Dietary risks were calculated in the above table for the U.S. general population and for those groups exposed to the highest risk. The chronic analyses were below the Agency's level of concern for all of the Population Subgroups using the Agency DEEM. The most highly exposed group was children 1-2 years old with 71.2% of the cPAD).

These residue calculations provide an acceptable dietary risk of concern for population subgroups for this chemical.

Issues That Must Be Resolved

I. For the 40 CFR 180.940 Regulations for sanitizing solutions:

Many of the labels include uses for the sanitization of food serving equipment, glasses, dishes, utensils and pots and pans. These surfaces that have been treated with the dodecylbenzene sulfonate products may bear small residues of the dodecylbenzene sulfonate Residues from treated surfaces can migrate to food coming into contact with the treated surfaces and can be ingested by humans.

Benzenesulfonic acid, dodecyl-: 40 CFR 180.940(c)

The site reads: "Food-processing equipment and utensils". The use limitation is 400 ppm.

Benzenesulfonic acid dodecyl-, sodium salt: 40 CFR 180.940(c)

The site reads, "Food processing equipment and utensils". The use limitation is 430 ppm equivalent to ~ 400ppm of the free acid.

Benzenesulfonic acid, dodecyl- : 40 CFR 180.940(b)

The site reads: “Dairy processing equipment, and food processing equipment and utensils”. The use limitation is 5.5 ppm.

It appears that dodecylbenzenesulfonic acid solutions containing up to 400 ppm can be used on dairy processing equipment and food processing equipment. The registrant and user may have difficulty in distinguishing between food processing equipment and dairy processing equipment. Many labels bear use directions with a treatment rate of greater than 5.5 ppm for dairy processing equipment.

Also, these 40 CFR citations also do not specifically state that the solutions may be used on food contact articles including dishes, pots and pans, glasses etc. However, there are many labels registered for use on these sites.

The Chemical Review Manager should ascertain the correct use sites and limitations for these chemicals.